

# On PPT States in $\mathcal{C}^K \otimes \mathcal{C}^M \otimes \mathcal{C}^N$ Composite Quantum Systems

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## Abstract

We study the general representations of positive partial transpose (PPT) states in  $\mathcal{C}^K \otimes \mathcal{C}^M \otimes \mathcal{C}^N$ . For the PPT states with rank- $N$  a canonical form is obtained, from which a sufficient separability condition is presented.

Key words: Separability, Quantum entanglement, PPT state

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Due to the importance of quantum entangled states in quantum information and computation [1, 2, 3], much effort has been done recently towards an operational characterization of separable states [4, 5, 6]. The manifestations of mixed-state entanglement can be very subtle [7]. Till now there is no general efficient criterion in judging the separability. The Bell inequalities [8], Peres PPT criterion [9], reduction criterion [10, 11], majorization [12], entanglement witnesses [13, 14], extension of Peres criterion [15], matrix realignment [16], generalized partial transposition criterion (GPT) [17], generalized reduced criterion [18], give some necessary (and also sufficient for some special cases [13]) conditions for separability. The separability criterion in [13] is both necessary and sufficient but not operational. For low rank density matrices there are also some necessary and sufficient operational criteria of separability [19, 20].

In [21, 22] the separability and entanglement of quantum mixed states in  $\mathcal{C}^2 \otimes \mathcal{C}^2 \otimes \mathcal{C}^N$ ,  $\mathcal{C}^2 \otimes \mathcal{C}^3 \otimes \mathcal{C}^N$  and  $\mathcal{C}^2 \otimes \mathcal{C}^2 \otimes \mathcal{C}^2 \otimes \mathcal{C}^N$  composite quantum systems have been studied in terms of matrix analysis on tensor spaces. It is shown that all such quantum states  $\rho$  with positive partial transposes and rank  $r(\rho) \leq N$  are separable. In this article we extend the results in [21] to the case of composite quantum systems in  $\mathcal{C}^K \otimes \mathcal{C}^M \otimes \mathcal{C}^N$  with general dimensions  $K, M, N \in \mathbb{N}$ . We give a canonical form of PPT states in  $\mathcal{C}^K \otimes \mathcal{C}^M \otimes \mathcal{C}^N$  with rank  $N$  and present a sufficient separability criterion.

A separable state in  $\mathcal{C}_A^K \otimes \mathcal{C}_B^M \otimes \mathcal{C}_C^N$  is of the form:

$$\rho_{ABC} = \sum_i p_i \rho_A^i \otimes \rho_B^i \otimes \rho_C^i, \quad (1)$$

where  $\sum_i p_i = 1$ ,  $0 < p_i \leq 1$ ,  $\rho_\alpha^i$  are density matrices associated with the subsystems  $\alpha$ ,  $\alpha = A, B, C$ . In the following we denote by  $R(\rho)$ ,  $K(\rho)$ ,  $r(\rho)$  and  $k(\rho)$  the range, kernel, rank and the dimension of the kernel of  $\rho$ , respectively.

We first derive a canonical form of PPT states in  $\mathcal{C}_A^3 \otimes \mathcal{C}_B^3 \otimes \mathcal{C}_C^N$  with rank  $N$ , which allows for an explicit decomposition of a given state in terms of convex sum of projectors on product vectors. Let  $|0_A\rangle, |1_A\rangle, |2_A\rangle; |0_B\rangle, |1_B\rangle, |2_B\rangle$ ; and  $|0_C\rangle \cdots |N-1_C\rangle$  be some local bases of the sub-systems A, B, C respectively.

**Lemma 1.** Every PPT state  $\rho$  in  $\mathcal{C}_A^3 \otimes \mathcal{C}_B^3 \otimes \mathcal{C}_C^N$  such that  $r(\langle 2_A, 2_B | \rho | 2_A, 2_B \rangle) = r(\rho) = N$ , can be transformed into the following canonical form by using a reversible local operation:

$$\rho = \sqrt{F} [DB \ DA \ D \ CB \ CA \ C \ B \ A \ I]^\dagger [DB \ DA \ D \ CB \ CA \ C \ B \ A \ I] \sqrt{F} \quad (2)$$

where  $A, B, C, D, F$  and the identity  $I$  are  $N \times N$  matrices acting on  $\mathcal{C}_C^N$  and satisfy the following relations:  $[A, A^\dagger] = [B, B^\dagger] = [C, C^\dagger] = [D, D^\dagger] = [B, A] = [B, A^\dagger] = [C, A] = [C, A^\dagger] = [D, A] = [D, A^\dagger] = [C, B] = [C, B^\dagger] = [D, B] = [D, B^\dagger] = [D, C] = [D, C^\dagger] = 0$  and  $F = F^\dagger$  ( $\dagger$  stands for the transposition and conjugate).

**Proof.** In the basis we considered, a density matrix  $\rho$  in  $\mathcal{C}_A^3 \otimes \mathcal{C}_B^3 \otimes \mathcal{C}_C^N$  with rank  $N$  can be always written as:

$$\rho = \begin{pmatrix} E_1 & E_{12} & E_{13} & E_{14} & E_{15} & E_{16} & E_{17} & E_{18} & E_{19} \\ E_{12}^\dagger & E_2 & E_{23} & E_{24} & E_{25} & E_{26} & E_{27} & E_{28} & E_{29} \\ E_{13}^\dagger & E_{23}^\dagger & E_3 & E_{34} & E_{35} & E_{36} & E_{37} & E_{38} & E_{39} \\ E_{14}^\dagger & E_{24}^\dagger & E_{34}^\dagger & E_4 & E_{45} & E_{46} & E_{47} & E_{48} & E_{49} \\ E_{15}^\dagger & E_{25}^\dagger & E_{35}^\dagger & E_{45}^\dagger & E_5 & E_{56} & E_{57} & E_{58} & E_{59} \\ E_{16}^\dagger & E_{26}^\dagger & E_{36}^\dagger & E_{46}^\dagger & E_{56}^\dagger & E_6 & E_{67} & E_{68} & E_{69} \\ E_{17}^\dagger & E_{27}^\dagger & E_{37}^\dagger & E_{47}^\dagger & E_{57}^\dagger & E_{67}^\dagger & E_7 & E_{78} & E_{79} \\ E_{18}^\dagger & E_{28}^\dagger & E_{38}^\dagger & E_{48}^\dagger & E_{58}^\dagger & E_{68}^\dagger & E_{78}^\dagger & E_8 & E_{89} \\ E_{19}^\dagger & E_{29}^\dagger & E_{39}^\dagger & E_{49}^\dagger & E_{59}^\dagger & E_{69}^\dagger & E_{79}^\dagger & E_{89}^\dagger & E_9 \end{pmatrix}, \quad (3)$$

where  $E'_s$  are  $N \times N$  matrices,  $r(E_9) = N$ . The projection  $\langle 2_A | \rho | 2_A \rangle$  gives rise to a state

$$\tilde{\rho} = \langle 2_A | \rho | 2_A \rangle = \begin{pmatrix} E_7 & E_{78} & E_{79} \\ E_{78}^\dagger & E_8 & E_{89} \\ E_{79}^\dagger & E_{89}^\dagger & E_9 \end{pmatrix}, \quad (4)$$

which is a state in  $\mathcal{C}_B^3 \otimes \mathcal{C}_C^N$  with  $r(\tilde{\rho}) = r(\rho) = N$ . Let  $t_\alpha$  denote the partial transposition with respect to the subsystem  $\alpha$ . As every principal minor determinant of  $\tilde{\rho}^{t_B}$  ( $\tilde{\rho}^{t_C}$ ) is some principal minor determinant of  $\rho$ , the fact that  $\rho$  is PPT implies that  $\tilde{\rho}$  is also PPT, i.e.,  $\tilde{\rho} \geq 0$ . After performing a reversible local non-unitary "filtering"  $\frac{1}{\sqrt{E_9}}$  on the third system and using Lemma 4 in [19] the matrix  $\tilde{\rho}$  can be written as

$$\tilde{\rho} = \begin{pmatrix} B^\dagger B & B^\dagger A & B^\dagger \\ A^\dagger B & A^\dagger A & A^\dagger \\ B & A & I \end{pmatrix}, \quad (5)$$

where  $[A, A^\dagger] = [B, B^\dagger] = [B, A] = [B, A^\dagger] = 0$ .

Similarly, if we consider the projection  $\langle 2_B | \rho | 2_B \rangle$ , for the same reasons as above we conclude that the resulting matrix

$$\begin{aligned}\bar{\rho} &= \langle 2_B | \rho | 2_B \rangle \\ &= \begin{pmatrix} E_3 & E_{36} & E_{39} \\ E_{36}^\dagger & E_6 & E_{69} \\ E_{39}^\dagger & E_{69}^\dagger & E_9 \end{pmatrix} = \begin{pmatrix} D^\dagger D & D^\dagger C & D^\dagger \\ C^\dagger D & C^\dagger C & C^\dagger \\ D & C & I \end{pmatrix},\end{aligned}$$

where  $[C, C^\dagger] = [D, D^\dagger] = [D, C] = [D, C^\dagger] = 0$ .

Summarizing, after performing a local filtering operation  $\frac{1}{\sqrt{E_9}}$  we can bring the matrix  $\rho$  to the form:

$$\rho = \begin{pmatrix} E_1 & E_{12} & E_{13} & E_{14} & E_{15} & E_{16} & E_{17} & E_{18} & E_{19} \\ E_{12}^\dagger & E_2 & E_{23} & E_{24} & E_{25} & E_{26} & E_{27} & E_{28} & E_{29} \\ E_{13}^\dagger & E_{23}^\dagger & D^\dagger D & E_{34} & E_{35} & D^\dagger C & E_{37} & E_{38} & D^\dagger \\ E_{14}^\dagger & E_{24}^\dagger & E_{34}^\dagger & E_4 & E_{45} & E_{46} & E_{47} & E_{48} & E_{49} \\ E_{15}^\dagger & E_{25}^\dagger & E_{35}^\dagger & E_{45}^\dagger & E_5 & E_{56} & E_{57} & E_{58} & E_{59} \\ E_{16}^\dagger & E_{26}^\dagger & C^\dagger D & E_{46}^\dagger & E_{56}^\dagger & C^\dagger C & E_{67} & E_{68} & C^\dagger \\ E_{17}^\dagger & E_{27}^\dagger & E_{37}^\dagger & E_{47}^\dagger & E_{57}^\dagger & E_{67}^\dagger & B^\dagger B & B^\dagger A & B^\dagger \\ E_{18}^\dagger & E_{28}^\dagger & E_{38}^\dagger & E_{48}^\dagger & E_{58}^\dagger & E_{68}^\dagger & A^\dagger B & A^\dagger A & A^\dagger \\ E_{19}^\dagger & E_{29}^\dagger & D & E_{49}^\dagger & E_{59}^\dagger & C & B & A & I \end{pmatrix}. \quad (6)$$

Notice that  $\langle \Psi_f | \rho | \Psi_f \rangle = 0$  for  $|\Psi_f\rangle = |21\rangle|f\rangle - |22\rangle A|f\rangle$  and arbitrary  $|f\rangle \in \mathcal{C}_C^N$ . As  $\rho \geq 0$  we have that  $|\Psi_f\rangle$  is in the kernel. Using the same method, we can get that  $\rho$  has the following kernel vectors:

$$\begin{aligned} &|21\rangle|f\rangle - |22\rangle A|f\rangle, \quad |20\rangle|g\rangle - |22\rangle B|g\rangle, \\ &|12\rangle|h\rangle - |22\rangle C|h\rangle, \quad |02\rangle|k\rangle - |22\rangle D|k\rangle, \end{aligned} \quad (7)$$

for all vectors  $|f\rangle, |g\rangle, |h\rangle, |k\rangle \in \mathcal{C}_C^N$ . This implies

$$\begin{aligned} E_{38} &= D^\dagger A, & E_{68} &= C^\dagger A, & E_{37} &= D^\dagger B, \\ E_{67} &= C^\dagger B, & E_{13} &= E_{19} D, & E_{23} &= E_{29} D, \\ E_{34}^\dagger &= E_{49} D, & E_{35}^\dagger &= E_{59} D, & E_{i6} &= E_{i9} C, \\ E_{i7} &= E_{i9} B, & E_{i8} &= E_{i9} A, & i &= 1, 2, 4, 5. \end{aligned} \quad (8)$$

Substituting (8) into (6) and considering partial transposition of  $\rho$  with respect to the first

sub-system A, we have

$$\rho^{t_A} = \begin{pmatrix} E_1 & E_{12} & E_{13} & E_{14}^\dagger & E_{24}^\dagger & E_{49}D & B^\dagger E_{19}^\dagger & B^\dagger E_{29}^\dagger & B^\dagger D \\ E_{12}^\dagger & E_2 & E_{23} & E_{15}^\dagger & E_{25}^\dagger & E_{59}D & A^\dagger E_{19}^\dagger & A^\dagger E_{29}^\dagger & A^\dagger D \\ E_{13}^\dagger & E_{23}^\dagger & D^\dagger D & C^\dagger E_{19}^\dagger & C^\dagger E_{29}^\dagger & C^\dagger D & E_{19}^\dagger & E_{29}^\dagger & D \\ E_{14} & E_{15} & E_{19}C & E_4 & E_{45} & E_{49}C & B^\dagger E_{49}^\dagger & B^\dagger E_{59}^\dagger & B^\dagger C \\ E_{24} & E_{25} & E_{29}C & E_{45}^\dagger & E_5 & E_{59}C & A^\dagger E_{49}^\dagger & A^\dagger E_{59}^\dagger & A^\dagger C \\ E_{34} & E_{35} & D^\dagger C & C^\dagger E_{49}^\dagger & C^\dagger E_{59}^\dagger & C^\dagger C & E_{49}^\dagger & E_{59}^\dagger & C \\ E_{19}B & E_{19}A & E_{19} & E_{49}B & E_{49}A & E_{49} & B^\dagger B & B^\dagger A & B^\dagger \\ E_{29}B & E_{29}A & E_{29} & E_{59}B & E_{59}A & E_{59} & A^\dagger B & A^\dagger A & A^\dagger \\ D^\dagger B & D^\dagger A & D^\dagger & C^\dagger B & C^\dagger A & C^\dagger & B & A & I \end{pmatrix}. \quad (9)$$

Since the partial transposition with respect to the sub-system A is positive,  $\rho^{t_A} \geq 0$ , and it does not change  $\langle 2_A | \rho | 2_A \rangle$ , we still have  $|20\rangle|g\rangle - |22\rangle B|g\rangle$ ,  $|21\rangle|f\rangle - |22\rangle A|f\rangle \in k(\rho^{t_A})$ . This gives rise to the following equalities:

$$\begin{aligned} E_{19} &= B^\dagger D^\dagger, & E_{29} &= A^\dagger D^\dagger, \\ E_{49} &= B^\dagger C^\dagger, & E_{59} &= A^\dagger C^\dagger. \end{aligned} \quad (10)$$

$\rho$  is then of the following form:

$$\begin{pmatrix} E_1 & E_{12} & B^\dagger D^\dagger D & E_{14} & E_{15} & B^\dagger D^\dagger C & B^\dagger D^\dagger B & B^\dagger D^\dagger A & B^\dagger D^\dagger \\ E_{12}^\dagger & E_2 & A^\dagger D^\dagger D & E_{24} & E_{25} & A^\dagger D^\dagger C & A^\dagger D^\dagger B & A^\dagger D^\dagger A & A^\dagger D^\dagger \\ D^\dagger DB & D^\dagger DA & D^\dagger D & D^\dagger CB & D^\dagger CA & D^\dagger C & D^\dagger B & D^\dagger A & D^\dagger \\ E_{14}^\dagger & E_{24}^\dagger & B^\dagger C^\dagger D & E_4 & E_{45} & B^\dagger C^\dagger C & B^\dagger C^\dagger B & B^\dagger C^\dagger A & B^\dagger C^\dagger \\ E_{15}^\dagger & E_{25}^\dagger & A^\dagger C^\dagger D & E_{45}^\dagger & E_5 & A^\dagger C^\dagger C & A^\dagger C^\dagger B & A^\dagger C^\dagger A & A^\dagger C^\dagger \\ C^\dagger DB & C^\dagger DA & C^\dagger D & C^\dagger CB & C^\dagger CA & C^\dagger C & C^\dagger B & C^\dagger A & C^\dagger \\ B^\dagger DB & B^\dagger DA & B^\dagger D & B^\dagger CB & B^\dagger CA & B^\dagger C & B^\dagger B & B^\dagger A & B^\dagger \\ A^\dagger DB & A^\dagger DA & A^\dagger D & A^\dagger CB & A^\dagger CA & A^\dagger C & A^\dagger B & A^\dagger A & A^\dagger \\ DB & DA & D & CB & CA & C & B & A & I \end{pmatrix}. \quad (11)$$

Set

$$X = \begin{pmatrix} E_{15} & B^\dagger D^\dagger C & B^\dagger D^\dagger B & B^\dagger D^\dagger A & B^\dagger D^\dagger \\ E_{25} & A^\dagger D^\dagger C & A^\dagger D^\dagger B & A^\dagger D^\dagger A & A^\dagger D^\dagger \\ D^\dagger CA & D^\dagger C & D^\dagger B & D^\dagger A & D^\dagger \\ E_{45} & B^\dagger C^\dagger C & B^\dagger C^\dagger B & B^\dagger C^\dagger A & B^\dagger C^\dagger \end{pmatrix},$$

$$Y = \begin{pmatrix} E_1 & E_{12} & B^\dagger D^\dagger D & E_{14} \\ E_{12}^\dagger & E_2 & A^\dagger D^\dagger D & E_{24} \\ D^\dagger DB & D^\dagger DA & D^\dagger D & D^\dagger CB \\ E_{14}^\dagger & E_{24}^\dagger & B^\dagger C^\dagger D & E_4 \end{pmatrix}$$

and

$$\rho_5 = \Sigma + \text{diag}(\Delta, 0, 0, 0, 0),$$

where

$$\Sigma = \begin{pmatrix} A^\dagger C^\dagger C A & A^\dagger C^\dagger C & A^\dagger C^\dagger B & A^\dagger C^\dagger A & A^\dagger C^\dagger \\ C^\dagger C A & C^\dagger C & C^\dagger B & C^\dagger A & C^\dagger \\ B^\dagger C A & B^\dagger C & B^\dagger B & B^\dagger A & B^\dagger \\ A^\dagger C A & A^\dagger C & A^\dagger B & A^\dagger A & A^\dagger \\ C A & C & B & A & I \end{pmatrix},$$

$$\Delta = E_5 - A^\dagger C^\dagger C A \quad (12)$$

and  $\text{diag}(A_1, A_2, \dots, A_m)$  denotes a diagonal block matrix with blocks  $A_1, A_2, \dots, A_m$ .  $\rho$  can then be written in the following partitioned matrix form:

$$\rho = \begin{pmatrix} Y & X \\ X^\dagger & \rho_5 \end{pmatrix}.$$

As  $\Sigma$  possesses the following  $4N$  kernel vectors:

$$\begin{aligned} & (\langle f|, 0, 0, 0, -\langle f|A^\dagger C^\dagger)^T, \quad (0, \langle g|, 0, 0, -\langle g|C^\dagger)^T, \\ & (0, 0, \langle h|, 0, -\langle h|B^\dagger)^T, \quad (0, 0, 0, \langle i|, -\langle i|A^\dagger)^T \end{aligned}$$

for arbitrary  $|f\rangle, |g\rangle, |h\rangle, |i\rangle \in \mathcal{C}_C^N$ , the kernel  $K(\Sigma)$  has at least dimension  $4N$ . On the other hand  $r(\Sigma) + k(\Sigma) = 5N$ , therefore  $r(\Sigma) \leq N$ . As the range of  $\Sigma$  has at least dimension  $N$  due to the identity entry on the diagonal, we have  $r(\Sigma) = N$ . Notice that  $r(\rho_5) \leq r(\rho) = N$ , it is easy to see that  $r(\rho_5) = N$ . To show that  $\Delta = 0$ , we make the following elementary row transformations on the matrix  $\rho_5$ ,

$$\begin{pmatrix} I & 0 & 0 & 0 & -A^\dagger C^\dagger \\ 0 & I & 0 & 0 & -C^\dagger \\ 0 & 0 & I & 0 & -B^\dagger \\ 0 & 0 & 0 & I & -A^\dagger \\ 0 & 0 & 0 & 0 & I \end{pmatrix} \rho_5 = \begin{pmatrix} \Delta & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ C A & C & B & A & I \end{pmatrix}. \quad (13)$$

As the rank of  $\rho_5$  is  $N$ , from (13) we have  $\Delta = 0$ , and hence  $E_5 = A^\dagger C^\dagger C A$ .

Now, notice that  $\langle \Psi_f | \rho | \Psi_f \rangle = 0$  for  $|\Psi_f\rangle = |11\rangle|f\rangle - |22\rangle C A |f\rangle$  and arbitrary  $|f\rangle \in \mathcal{C}_C^N$ . Since  $\rho \geq 0$  we have  $0 = \rho |\Psi_f\rangle = |00\rangle(E_{15} - B^\dagger D^\dagger C A)|f\rangle + |01\rangle(E_{25} - A^\dagger D^\dagger C A)|f\rangle + |10\rangle(E_{45} - B^\dagger C^\dagger C A)|f\rangle$ , which, as  $|f\rangle$  is arbitray, leads to  $E_{15} = B^\dagger D^\dagger C A$ ,  $E_{25} = A^\dagger D^\dagger C A$ ,  $E_{45} = B^\dagger C^\dagger C A$ , thus the matrix  $\rho$  becomes

$$\begin{pmatrix} E_1 & E_{12} & B^\dagger D^\dagger D & E_{14} & B^\dagger D^\dagger C A & B^\dagger D^\dagger C & B^\dagger D^\dagger B & B^\dagger D^\dagger A & B^\dagger D^\dagger \\ E_{12}^\dagger & E_2 & A^\dagger D^\dagger D & E_{24} & A^\dagger D^\dagger C A & A^\dagger D^\dagger C & A^\dagger D^\dagger B & A^\dagger D^\dagger A & A^\dagger D^\dagger \\ D^\dagger D B & D^\dagger D A & D^\dagger D & D^\dagger C B & D^\dagger C A & D^\dagger C & D^\dagger B & D^\dagger A & D^\dagger \\ E_{14}^\dagger & E_{24}^\dagger & B^\dagger C^\dagger D & E_4 & B^\dagger C^\dagger C A & B^\dagger C^\dagger C & B^\dagger C^\dagger B & B^\dagger C^\dagger A & B^\dagger C^\dagger \\ A^\dagger C^\dagger D B & A^\dagger C^\dagger D A & A^\dagger C^\dagger D & A^\dagger C^\dagger C B & A^\dagger C^\dagger C A & A^\dagger C^\dagger C & A^\dagger C^\dagger B & A^\dagger C^\dagger A & A^\dagger C^\dagger \\ C^\dagger D B & C^\dagger D A & C^\dagger D & C^\dagger C B & C^\dagger C A & C^\dagger C & C^\dagger B & C^\dagger A & C^\dagger \\ B^\dagger D B & B^\dagger D A & B^\dagger D & B^\dagger C B & B^\dagger C A & B^\dagger C & B^\dagger B & B^\dagger A & B^\dagger \\ A^\dagger D B & A^\dagger D A & A^\dagger D & A^\dagger C B & A^\dagger C A & A^\dagger C & A^\dagger B & A^\dagger A & A^\dagger \\ D B & D A & D & C B & C A & C & B & A & I \end{pmatrix}. \quad (14)$$

Similarly, we can derive  $E_4 = B^\dagger C^\dagger CB$ ,  $E_{14} = B^\dagger D^\dagger CB$ ,  $E_{24} = A^\dagger D^\dagger CB$ ,  $E_2 = A^\dagger D^\dagger DA$ ,  $E_{12} = B^\dagger D^\dagger DA$ ,  $E_1 = B^\dagger D^\dagger DB$ .  $\rho$  then is of the following form:

$$\begin{pmatrix} B^\dagger D^\dagger DB & B^\dagger D^\dagger DA & B^\dagger D^\dagger D & B^\dagger D^\dagger CB & B^\dagger D^\dagger CA & B^\dagger D^\dagger C & B^\dagger D^\dagger B & B^\dagger D^\dagger A & B^\dagger D^\dagger \\ A^\dagger D^\dagger DB & A^\dagger D^\dagger DA & A^\dagger D^\dagger D & A^\dagger D^\dagger CB & A^\dagger D^\dagger CA & A^\dagger D^\dagger C & A^\dagger D^\dagger B & A^\dagger D^\dagger A & A^\dagger D^\dagger \\ D^\dagger DB & D^\dagger DA & D^\dagger D & D^\dagger CB & D^\dagger CA & D^\dagger C & D^\dagger B & D^\dagger A & D^\dagger \\ B^\dagger C^\dagger DB & B^\dagger C^\dagger DA & B^\dagger C^\dagger D & B^\dagger C^\dagger CB & B^\dagger C^\dagger CA & B^\dagger C^\dagger C & B^\dagger C^\dagger B & B^\dagger C^\dagger A & B^\dagger C^\dagger \\ A^\dagger C^\dagger DB & A^\dagger C^\dagger DA & A^\dagger C^\dagger D & A^\dagger C^\dagger CB & A^\dagger C^\dagger CA & A^\dagger C^\dagger C & A^\dagger C^\dagger B & A^\dagger C^\dagger A & A^\dagger C^\dagger \\ C^\dagger DB & C^\dagger DA & C^\dagger D & C^\dagger CB & C^\dagger CA & C^\dagger C & C^\dagger B & C^\dagger A & C^\dagger \\ B^\dagger DB & B^\dagger DA & B^\dagger D & B^\dagger CB & B^\dagger CA & B^\dagger C & B^\dagger B & B^\dagger A & B^\dagger \\ A^\dagger DB & A^\dagger DA & A^\dagger D & A^\dagger CB & A^\dagger CA & A^\dagger C & A^\dagger B & A^\dagger A & A^\dagger \\ DB & DA & D & CB & CA & C & B & A & I \end{pmatrix} \\ = [DB \ DA \ D \ CB \ CA \ C \ B \ A \ I]^\dagger [DB \ DA \ D \ CB \ CA \ C \ B \ A \ I]$$

The commutative relations  $[A, D] = [B, D] = [A, C] = [B, C] = [A, D^\dagger] = [B, D^\dagger] = [A, C^\dagger] = [B, C^\dagger] = 0$  follow from the positivity of all partial transpositions of  $\rho$ . We first consider:

$$\rho^{t_B} = \begin{pmatrix} B^\dagger D^\dagger DB & A^\dagger D^\dagger DB & D^\dagger DB & B^\dagger D^\dagger CB & A^\dagger D^\dagger CB & D^\dagger CB & B^\dagger D^\dagger B & A^\dagger D^\dagger B & D^\dagger B \\ B^\dagger D^\dagger DA & A^\dagger D^\dagger DA & D^\dagger DA & B^\dagger D^\dagger CA & A^\dagger D^\dagger CA & D^\dagger CA & B^\dagger D^\dagger A & A^\dagger D^\dagger A & D^\dagger A \\ B^\dagger D^\dagger D & A^\dagger D^\dagger D & D^\dagger D & B^\dagger D^\dagger C & A^\dagger D^\dagger C & D^\dagger C & B^\dagger D^\dagger & A^\dagger D^\dagger & D^\dagger \\ B^\dagger C^\dagger DB & A^\dagger C^\dagger DB & C^\dagger DB & B^\dagger C^\dagger CB & A^\dagger C^\dagger CB & C^\dagger CB & B^\dagger C^\dagger B & A^\dagger C^\dagger B & C^\dagger B \\ B^\dagger C^\dagger DA & A^\dagger C^\dagger DA & C^\dagger DA & B^\dagger C^\dagger CA & A^\dagger C^\dagger CA & C^\dagger CA & B^\dagger C^\dagger A & A^\dagger C^\dagger A & C^\dagger A \\ B^\dagger C^\dagger D & A^\dagger C^\dagger D & C^\dagger D & B^\dagger C^\dagger C & A^\dagger C^\dagger C & C^\dagger C & B^\dagger C^\dagger & A^\dagger C^\dagger & C^\dagger \\ B^\dagger DB & A^\dagger DB & DB & B^\dagger CB & A^\dagger CB & CB & B^\dagger B & A^\dagger B & B \\ B^\dagger DA & A^\dagger DA & DA & B^\dagger CA & A^\dagger CA & CA & B^\dagger A & A^\dagger A & A \\ B^\dagger D & A^\dagger D & D & B^\dagger C & A^\dagger C & C & B^\dagger & A^\dagger & I \end{pmatrix}$$

Due to the positivity, the matrix  $\rho^{t_B}$  must possess the kernel vector  $|12\rangle|f\rangle - |22\rangle C|f\rangle, |02\rangle|g\rangle - |22\rangle D|g\rangle$ , which implies that  $[A, C] = [B, C] = [A, D] = [B, D] = 0$ . The matrix  $\rho^{t_B}$  can be then written as:

$$\rho^{t_B} = \begin{pmatrix} D^\dagger B \\ D^\dagger A \\ D^\dagger \\ C^\dagger B \\ C^\dagger A \\ C^\dagger \\ C \\ B \\ A \\ I \end{pmatrix} \begin{pmatrix} B^\dagger D & A^\dagger D & D & B^\dagger C & A^\dagger C & C & B^\dagger & A^\dagger & I \end{pmatrix},$$

which implies automatically the positivity.

From the positivity of  $\rho^{tAB}$ ,

$$\rho^{tAB} = \begin{pmatrix} B^\dagger D^\dagger DB & A^\dagger D^\dagger DB & D^\dagger DB & B^\dagger C^\dagger DB & A^\dagger C^\dagger DB & C^\dagger DB & B^\dagger DB & A^\dagger DB & DB \\ B^\dagger D^\dagger DA & A^\dagger D^\dagger DA & D^\dagger DA & B^\dagger C^\dagger DA & A^\dagger C^\dagger DA & C^\dagger DA & B^\dagger DA & A^\dagger DA & DA \\ B^\dagger D^\dagger D & A^\dagger D^\dagger D & D^\dagger D & B^\dagger C^\dagger D & A^\dagger C^\dagger D & C^\dagger D & B^\dagger D & A^\dagger D & D \\ B^\dagger D^\dagger CB & A^\dagger D^\dagger CB & D^\dagger CB & B^\dagger C^\dagger CB & A^\dagger C^\dagger CB & C^\dagger CB & B^\dagger CB & A^\dagger CB & CB \\ B^\dagger D^\dagger CA & A^\dagger D^\dagger CA & D^\dagger CA & B^\dagger C^\dagger CA & A^\dagger C^\dagger CA & C^\dagger CA & B^\dagger CA & A^\dagger CA & CA \\ B^\dagger D^\dagger C & A^\dagger D^\dagger C & D^\dagger C & B^\dagger C^\dagger C & A^\dagger C^\dagger C & C^\dagger C & B^\dagger C & A^\dagger C & C \\ B^\dagger D^\dagger B & A^\dagger D^\dagger B & D^\dagger B & B^\dagger C^\dagger B & A^\dagger C^\dagger B & C^\dagger B & B^\dagger B & A^\dagger B & B \\ B^\dagger D^\dagger A & A^\dagger D^\dagger A & D^\dagger A & B^\dagger C^\dagger A & A^\dagger C^\dagger A & C^\dagger A & B^\dagger A & A^\dagger A & A \\ B^\dagger D^\dagger & A^\dagger D^\dagger & D^\dagger & B^\dagger C^\dagger & A^\dagger C^\dagger & C^\dagger & B^\dagger & A^\dagger & I \end{pmatrix},$$

we have that  $|12\rangle|f\rangle - |22\rangle C^\dagger|f\rangle$ ,  $|02\rangle|g\rangle - |22\rangle D^\dagger|g\rangle$  are kernel vectors, which results in  $[A, D^\dagger] = [B, D^\dagger] = [A, C^\dagger] = [B, C^\dagger] = 0$ .  $\rho^{tAB}$  is then of the form:

$$\rho^{tAB} = \begin{pmatrix} DB \\ DA \\ D \\ CB \\ CA \\ C \\ B \\ A \\ I \end{pmatrix} \begin{pmatrix} B^\dagger D^\dagger & A^\dagger D^\dagger & D^\dagger & B^\dagger C^\dagger & A^\dagger C^\dagger & C^\dagger & B^\dagger & A^\dagger & I \end{pmatrix}.$$

This form assures positive definiteness, and concludes the proof of the Lemma.  $\square$

Using Lemma 1 we can prove the following Theorem:

**Theorem 1.** A PPT-state  $\rho$  in  $\mathcal{C}^3 \otimes \mathcal{C}^3 \otimes \mathcal{C}^N$  with  $r(\rho) = N$  is separable if there exists a product basis  $|e_A, f_B\rangle$  such that  $r(\langle e_A, f_B | \rho | e_A, f_B \rangle) = N$ .

**Proof.** According to the Lemma the PPT state  $\rho$  can be written as

$$\rho = \begin{pmatrix} B^\dagger D^\dagger \\ A^\dagger D^\dagger \\ D^\dagger \\ B^\dagger C^\dagger \\ A^\dagger C^\dagger \\ C^\dagger \\ B^\dagger \\ A^\dagger \\ I \end{pmatrix} \begin{pmatrix} DB & DA & D & CB & CA & C & B & A & I \end{pmatrix}.$$

Since all  $A, A^\dagger, B, B^\dagger, C, C^\dagger, D$  and  $D^\dagger$  commute, they have common eigenvectors  $|f_n\rangle$ . Let

$a_n, b_n, c_n$  and  $d_n$  be the corresponding eigenvalues of  $A, B, C$  and  $D$  respectively. We have

$$\begin{aligned} \langle f_n | \rho | f_n \rangle &= \begin{pmatrix} b_n^* d_n^* \\ a_n^* d_n^* \\ d_n^* \\ b_n^* c_n^* \\ a_n^* c_n^* \\ c_n^* \\ b_n^* \\ a_n^* \\ 1 \end{pmatrix} \begin{pmatrix} d_n b_n & d_n a_n & d_n & c_n b_n & c_n a_n & c_n & b_n & a_n & 1 \end{pmatrix} \\ &= \left[ \begin{pmatrix} d_n^* \\ c_n^* \\ 1 \end{pmatrix} \otimes \begin{pmatrix} b_n^* \\ a_n^* \\ 1 \end{pmatrix} \right] (d_n \ c_n \ 1) \otimes (b_n \ a_n \ 1) = |e_A, f_B\rangle \langle e_A, f_B|. \end{aligned}$$

We can thus write  $\rho$  as

$$\rho = \sum_{n=1}^N |\psi_n\rangle \langle \psi_n| \otimes |\phi_n\rangle \langle \phi_n| \otimes |f_n\rangle \langle f_n|,$$

where

$$|\psi_n\rangle = \begin{pmatrix} d_n^* \\ c_n^* \\ 1 \end{pmatrix}, \quad |\phi_n\rangle = \begin{pmatrix} b_n^* \\ a_n^* \\ 1 \end{pmatrix}.$$

Because the local transformations are reversible, we can now apply the inverse transformations and obtain a decomposition of the initial state  $\rho$  in a sum of projectors onto product vectors. This proves the separability of  $\rho$ .  $\square$

The above approach can be extended to the case of higher dimensions like  $\mathcal{C}_A^3 \otimes \mathcal{C}_B^M \otimes \mathcal{C}_C^N$ . Let  $|0_A\rangle, |1_A\rangle, |2_A\rangle; |0_B\rangle, \dots, |M-1_B\rangle$ ; and  $|0_C\rangle \dots |N-1_C\rangle$  be some local bases of the sub-systems A, B, C respectively. From Lemma 1 it is straightforward to prove the following conclusion:

**Lemma 2.** Every PPT state  $\rho$  in  $\mathcal{C}_A^3 \otimes \mathcal{C}_B^M \otimes \mathcal{C}_C^N$  such that  $r(\langle 2_A, M-1_B | \rho | 2_A, M-1_B \rangle) = r(\rho) = N$ , can be transformed into the following canonical form by using a reversible local operation:

$$\rho = \sqrt{F} T^\dagger T \sqrt{F}, \quad (15)$$

where  $T = (C \ B \ I) \otimes (A_{M-1} \ A_{M-2} \ \dots \ A_1 \ I)$ ,  $A_i, B, C, F$  and the identity  $I$  are  $N \times N$  matrices acting on  $\mathcal{C}_C^N$  and satisfy the following relations:  $[A_i, A_j] = [A_i, A_j^\dagger] = [B, B^\dagger] = [C, C^\dagger] = [B, A_i] = [B, A_i^\dagger] = [C, A_i] = [C, A_i^\dagger] = 0$ ,  $i, j = 1, 2, \dots, M-1$  and  $F = F^\dagger$ .

Extending Theorem 1 to higher dimensions, we have:

**Theorem 2.** A PPT-state  $\rho$  in  $\mathcal{C}^3 \otimes \mathcal{C}^M \otimes \mathcal{C}^N$  with  $r(\rho) = N$  is separable if there exists a product basis  $|e_A, f_B\rangle$  such that  $r(\langle e_A, f_B | \rho | e_A, f_B \rangle) = N$ .



By extending Lemma 2, Theorem 2 and the results in [21] and [22], we can give the canonical form of PPT states in  $\mathcal{C}_A^K \otimes \mathcal{C}_B^M \otimes \mathcal{C}_C^N$  with rank  $N$ . Let  $|0_A\rangle, \dots, |K-1_A\rangle; |0_B\rangle, \dots, |M-1_B\rangle;$  and  $|0_C\rangle \dots |N-1_C\rangle$  be some local bases of the sub-systems A, B, C respectively.

**Lemma 3.** Every PPT state  $\rho$  in  $\mathcal{C}_A^K \otimes \mathcal{C}_B^M \otimes \mathcal{C}_C^N$  such that  $r(\langle K-1_A, M-1_B | \rho | K-1_A, M-1_B \rangle) = r(\rho) = N$ , can be transformed into the following canonical form by using a reversible local operation:

$$\rho = \sqrt{F} T^\dagger T \sqrt{F}, \quad (16)$$

where  $T = (B_{K-1} \ B_{K-2} \ \dots \ B_1 \ I) \otimes (A_{M-1} \ A_{M-2} \ \dots \ A_1 \ I)$ ,  $A_i, B_j, F$  and  $I$  are  $N \times N$  matrices acting on  $\mathcal{C}_C^N$  and satisfy the following relations:  $[A_i, A_s] = [A_i, A_s^\dagger] = [B_t, B_j] = [B_t, B_j^\dagger] = [A_i, B_j] = [A_i, B_j^\dagger] = 0$  and  $F = F^\dagger, i, s = 1, 2, \dots, M-1, j, t = 1, 2, \dots, K-1$ .

**Proof.** In the basis we considered, a density matrix  $\rho$  in  $\mathcal{C}_A^K \otimes \mathcal{C}_B^M \otimes \mathcal{C}_C^N$  with rank  $N$  can be always written as a  $KM \times KM$  partitioned matrix. Let  $E_{ij}$  be the  $i, j$ -element of  $\rho$ . Denote  $E_{ii} = E_i$ . Every  $E_i$ 's are  $N \times N$ -matrices and  $r(E_{KM}) = N$ . Because  $\rho$  is self-adjoint, we have  $E_{ij} = E_{ji}^\dagger, i > j$ .

The projection  $\langle K-1_A | \rho | K-1_A \rangle$  gives rise to a state  $\tilde{\rho} = \langle K-1_A | \rho | K-1_A \rangle$  which is a state in  $\mathcal{C}_B^M \otimes \mathcal{C}_C^N$  with  $r(\tilde{\rho}) = r(\rho) = N$ . The fact that  $\rho$  is PPT implies that  $\tilde{\rho}$  is also PPT, i.e.,  $\tilde{\rho} \geq 0$ . Using the Lemma 5 in [19] we have

$$\tilde{\rho} = [C_1, \dots, C_{M-1}, I]^\dagger [C_1, \dots, C_{M-1}, I], \quad (17)$$

where  $[C_i, C_j^\dagger] = [C_i, C_j] = 0, i, j = 1, \dots, M-1$ .

Similarly, if we consider the projection  $\langle M-1_B | \rho | M-1_B \rangle$ , we have

$$\bar{\rho} = [D_1, \dots, D_{K-1}, I]^\dagger [D_1, \dots, D_{K-1}, I], \quad (18)$$

where  $[D_i, D_j^\dagger] = [D_i, D_j] = 0, i, j = 1, \dots, K-1$ . Altogether we have  $K^2 + M^2 - 1$   $E_i$ 's.

$\rho$  has the following  $M-1$  kernel vectors:

$$|K-1, i\rangle |f_i\rangle - |K-1, M-1\rangle C_{M-i-1} |f_i\rangle, \quad i = 0, 1, \dots, M-2 \quad (19)$$

for all vectors  $|f_i\rangle \in \mathcal{C}_C^N$ . Similarly there are  $K-1$  other kernel vectors,

$$|j, K-1\rangle |g_j\rangle - |K-1, M-1\rangle D_j |g_j\rangle, \quad j = 0, 1, \dots, K-2 \quad (20)$$

for all vectors  $|g_j\rangle \in \mathcal{C}_C^N$ . From these kernel vectors of  $\rho$ , we observe that the  $E_{ij}$  are dependent on the last column elements of  $\rho$ . From  $\rho^{t_A} \geq 0$  and that the partial transposition of  $\rho$  with respect to the first sub-system A does not change the positivity of  $\langle K-1_A | \rho | K-1_A \rangle$ , we still have some kernel vectors that belong to  $k(\rho^{t_A})$ , from which we can get the last column elements

and hence the last row elements of  $\rho$ . Then we can write  $\rho$  in the following partitioned matrix form:

$$\rho = \begin{pmatrix} Y & X \\ X^\dagger & \rho_0 \end{pmatrix}$$

with

$$\rho_0 = \begin{pmatrix} E_k & Z \\ Z^\dagger & W \end{pmatrix},$$

where  $Z$  and  $W$  are known,  $k = KM - (M + 1)$ . Similar to the proof of Lemma 1, denoting  $\rho_0 = \Sigma + \text{diag}(\Delta, 0, 0, \dots, 0)$  and proving that  $\Delta = 0$  we get the form of  $E_k$ .

By repeating the procedure above, we can calculate all the diagonal elements of  $\rho$ . The rest commuting relations among  $A_i, B_j$  can be obtained from the PPT properties of  $\rho$ , similar to the case in Lemma 1.  $\square$

From the canonical form (16), we can obtain the following result:

**Theorem 3.** A PPT-state  $\rho$  in  $\mathcal{C}^K \otimes \mathcal{C}^M \otimes \mathcal{C}^N$  with  $r(\rho) = N$  is separable if there exists a product basis  $|e_A, f_B\rangle$  such that  $r(\langle e_A, f_B | \rho | e_A, f_B \rangle) = N$ .

In the following we give some detailed examples related to our canonical form of PPT states and the separability criterion.

i) An obvious separable mixed state on  $K \times M \times N$  is  $\rho = \begin{pmatrix} \frac{1}{N}I & 0 \\ 0 & 0 \end{pmatrix}$ , where  $I$  is an  $N \times N$  unit matrix. Obviously  $\rho$  is a *PPT* state with rank  $N$ , and there exist  $|e_A\rangle = |0_A\rangle$ ,  $|f_B\rangle = |0_B\rangle$ , such that  $\langle e_A, f_B | \rho | e_A, f_B \rangle = \frac{1}{N}I$ . Therefore  $r(\langle e_A, f_B | \rho | e_A, f_B \rangle) = r(\rho) = N$ . Thus the conditions in Theorem 3 are satisfied and  $\rho$  is separable. In fact, if we set  $|\psi_1\rangle = |\psi_2\rangle = |0_A\rangle$ ,  $|\phi_1\rangle = |\phi_2\rangle = |0_B\rangle$ ,  $|\varphi_1\rangle = \frac{1}{\sqrt{2}}(|0_C\rangle + |1_C\rangle)$ ,  $|\varphi_2\rangle = \frac{1}{\sqrt{2}}(|0_C\rangle - |1_C\rangle)$ ,  $p_1 = p_2 = \frac{1}{2}$ , then  $\rho$  can be written in a separated form:

$$\rho = p_1 \rho_{11} \otimes \rho_{12} \otimes \rho_{13} + p_2 \rho_{21} \otimes \rho_{22} \otimes \rho_{23},$$

where  $\rho_{i1} = |\psi_i\rangle\langle\psi_i|$ ,  $\rho_{i2} = |\phi_i\rangle\langle\phi_i|$ ,  $\rho_{i3} = |\varphi_i\rangle\langle\varphi_i|$ ,  $i = 1, 2$ .

ii) Consider a three-qubit state:  $\rho = \begin{pmatrix} A & 0 \\ 0 & 0 \end{pmatrix}$  with  $A = \begin{pmatrix} \frac{1}{2} & a \\ a & \frac{1}{2} \end{pmatrix}$ ,  $a \in \mathbb{R}$ .  $\rho$  is a mixed state as  $\text{tr}\rho^2 < 1$ . It is easily verified that  $\rho$  is *PPT*:

$$\rho^{tA} = \rho^{tB} = \rho^{tC} = \rho^{tAB} = \rho^{tAC} = \rho^{tBC} = \rho$$

and  $r(\rho) = 2$ . Let  $|e_A\rangle = |f_B\rangle = |0\rangle$ . We have  $\langle e_A, f_B | \rho | e_A, f_B \rangle = \frac{1}{2}I$ . Therefore  $r(\langle e_A, f_B | \rho | e_A, f_B \rangle) = r(\rho) = 2$ . From Theorem 3  $\rho$  is separable. In fact  $\rho$  has separable form

$$\rho = p_1 \rho_{11} \otimes \rho_{12} \otimes \rho_{13} + p_2 \rho_{21} \otimes \rho_{22} \otimes \rho_{23},$$

where  $|\psi_1\rangle = |\psi_2\rangle = |\phi_1\rangle = |\phi_2\rangle = |0\rangle$ ,  $|\varphi_1\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ ,  $|\varphi_2\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$ ,  $p_1 = p_2 = \frac{1}{2}$ , and  $\rho_{i1} = |\psi_i\rangle\langle\psi_i|$ ,  $\rho_{i2} = |\phi_i\rangle\langle\phi_i|$ ,  $\rho_{i3} = |\varphi_i\rangle\langle\varphi_i|$ ,  $i = 1, 2$ .

iii) The biseparable three-qubit bound entangled state:

$$\rho = \frac{1}{8}(I - \sum_{i=1}^4 |\psi_i\rangle\langle\psi_i|),$$

where  $|\psi_i\rangle$ 's are given by  $|0, 1, +\rangle$ ,  $|1, +, 0\rangle$ ,  $|+, 1, 0\rangle$ ,  $|-, -, -\rangle$  with  $|\pm\rangle = \frac{1}{\sqrt{2}}(|0\rangle \pm |1\rangle)$ .  $\rho$  is a PPT state as  $\rho^{tA} = \rho^{tB} = \rho^{tC} = \rho^{tAB} = \rho^{tAC} = \rho^{tBC} = \rho$ . It is separable under any bipartite cut  $A|BC, B|AC, B|CA$ . But it is entangled (not fully separable). As  $r(\rho) \neq 2$  this state does not satisfy the conditions of Theorem 3 and the corresponding conclusions could not be deduced.

We have derived a canonical form of PPT states in  $\mathcal{C}^K \otimes \mathcal{C}^M \otimes \mathcal{C}^N$  with rank  $N$  and a sufficient separability criterion from this canonical form. For  $K \geq 2$ ,  $M \geq 3$ , the separability criterion we can deduce is weaker, as PPT criterion is no longer sufficient and necessary for the separability of bipartite states. Nevertheless the canonical representation of PPT states can shade light on studying the structure of bound entangled states which are PPT but not separable.

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